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The DOE Center of Excellence for The Synthesis and Processing of Advanced Materials

Basic Energy Sciences
Division of Materials Sciences and Engineering

http://www.sandia.gov/1100/XCSP/xcsp_homepage.htm

A model of integration within the DOE as well as of collaborations among the participating institutions

Center Review

Germantown, MD, June 3-4, 2004

OVERVIEW

Outline

- Center and its Objective
- Current Center Projects
- Recent Project Changes
- Some Reflections

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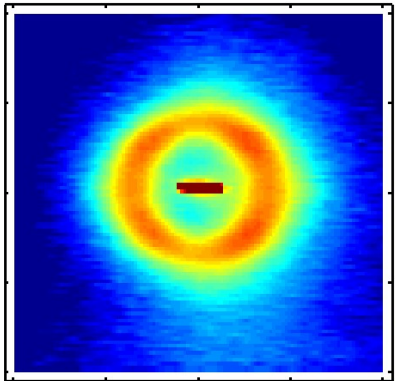
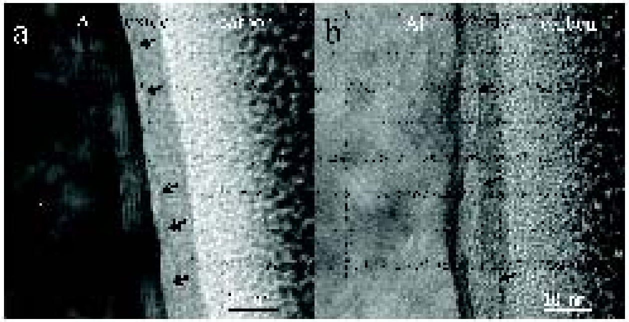
- A coordinated/cooperative venture among
  -12 DOE Labs
  -University Grant Research
  -Industrial Collaborators
- *Objective*
  To enhance the science and engineering of materials synthesis and processing in order to meet the programmatic needs of the Department of Energy and to facilitate the technological exploitation of materials.
- Capitalizes on the complementary strengths of the participating institutions to solve important problems and add value

Perovskite Thin Films



X-ray scattering from $PbTiO_3$ films

Localized Corrosion



Nano-void nucleation at the Al/Al_2O_3 interface

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Multi-Lab Center Projects Emphasize Scientific Excellence & Technological Relevance

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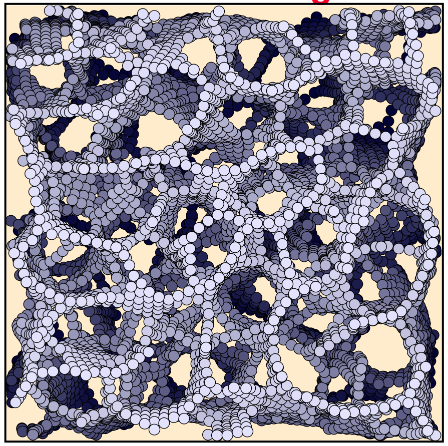
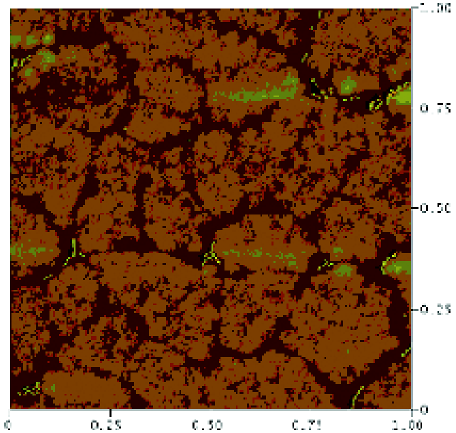
- Isolated and Collective Phenomena in Nanocomposite Magnets
- Controlled Defect Structures in Rare-Earth Ba-Cu-O Cuprate Superconductors
- Smart Structures Based on Electroactive Polymers
- Nanoscale Phenomena in Perovskite Thin Films
- Granular Flow and Kinetics
- Synthesis and Processing of Carbon-based Nanostructured Materials
- Experimental and Computational Lubrication at the Nanoscale
- Spin-Polarzied Transport in Complex Oxides

Nano-Scale Magnets



Simulated nanocomposites formed in a triaxial field

Carbon Nanostructures



AFM image of nano-crystalline diamond film

Center Projects

Selection Criteria

- Scientific excellence
- Clear relationship to energy-related technologies
- Involvement of several laboratories
- Existing or potential partnerships with DOE Technologies-funded programs
- Existing or potential in-kind partnerships with industry

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Center Projects Build on Selected Activities from On-Going Research Programs at the Laboratories

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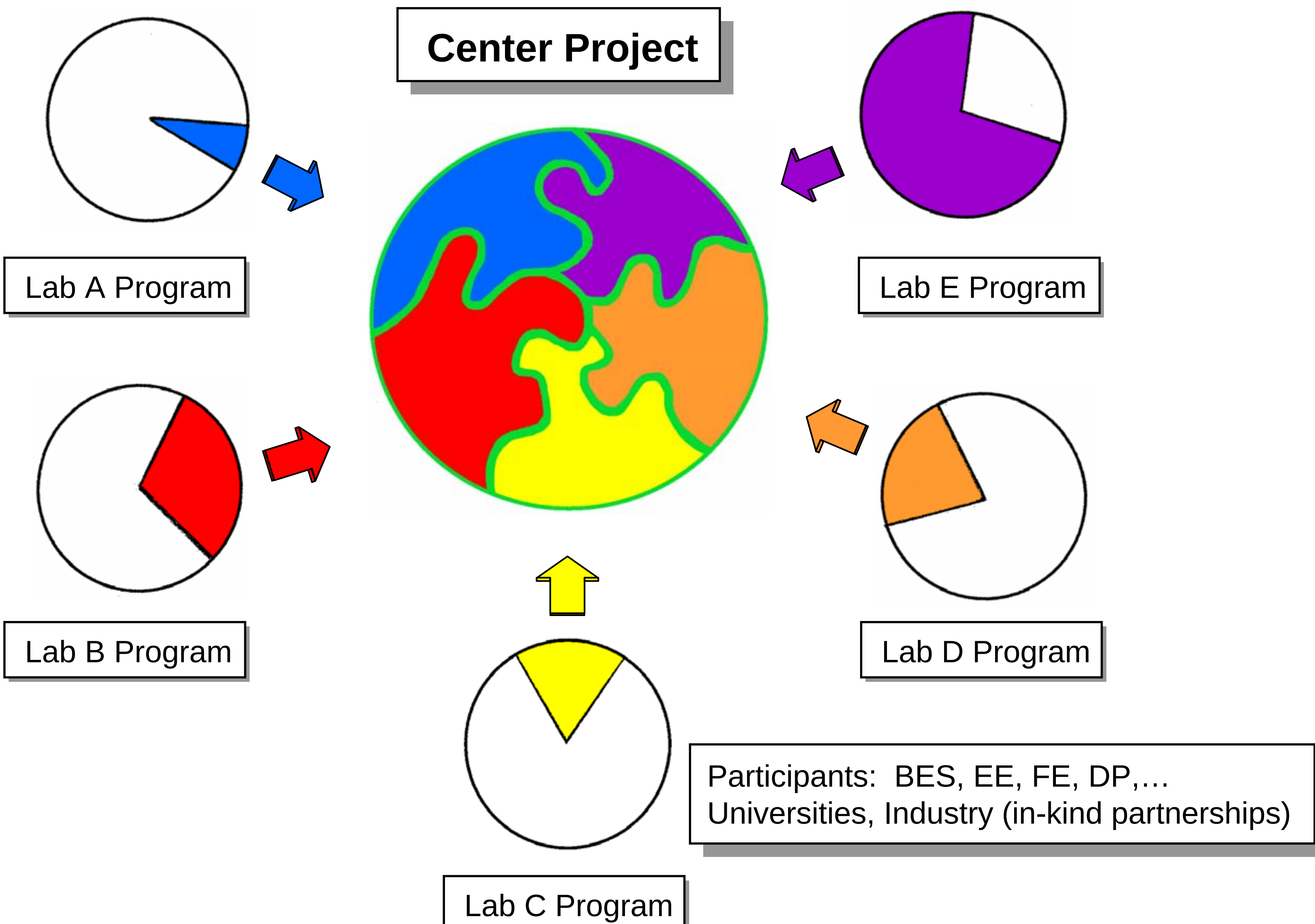

CSP PROJECTS FY'04 "Glue" Funding Summary

Lab \ Project	Nano Magnets	Cuprate Superconductors	Perovskite Films	Electroactive Polymers	Granular Flow	Carbon Nanostructures	Nanoscale Lubrication	Complex Oxides
Ames	25 (01-03) 25 (02-02)	30 (01-05)		8 (03-02)	110*[a] (02-03)			
ANL	65 (02-02)	60 (01-05)	145*[b] (01-03)	35 (03-01)	75 (02-02)	110*[c] (03-01)	20 (03-01)	80 (02-02)
BNL	35 (02-05)	65 (01-03)		25 (03-02)				30 (04-01)
INEEL				20 (01-05)				
UI/MRL	20 (01-03)			36 (02-02)			55 (01-03)	30 (02-02)
LBNL	25 (02-02)			5 (03-01)		28 (01-01)	30 (03-01)	30 (01-03) 30 (xx-xx)
LLNL	10 (03-01)			20 (02-03)				10 (03-01)
LANL	25 (01-05)	50 (02-01)	5 (02-02)	21(03-01)	70 (02-01)		20 (01-05)	60 (02-01)
NREL								
ORNL	25 (01-05)	60 (02-02)	80 (01-03)	30 (03-01)		67 (02-02)	55 (01-01)	30 (02-02)
PNNL				70*[d] (01-05)			25 (01-05)	
SNL/CA								
SNL/NM	20 (03-01)	35 (01-05)	35 (01-01)	30 (03-01)	45 (01-02)	67 (01-05)	55 (01-02) 15 (01-01)	
TOTAL ($K)	275*[e]	300	265*[f]	300	300	272*[g]	275 *[h]	300

[a] Includes $65 K for university grants and workshops.
[b] Include $10 K for Univ. of Florida, $15K for Univ. of Maryland, $10K UNC/CH, $15K for workshops.
[c] Includes $28 K subcontract to NCSU (Nemanich).
[d] Includes $25 K for university subcontract – B.I. Lee (Clemson)
[e] Remaining $25 K should be sent to Prof. Kannan Krishnan, University of Washington on his DMS&E contract.
[f] Remaining $35K should be sent directly to Prof. Dravid, Northwestern Univ. on DMS&E contract.
[g] Remaining 28K should be sent directly to Prof. Robert Carpic, Univ. of Wisconsin on DMS&E contract.
[h] Remaining $25 K should be sent directly to Prof. S. Sinha at UC/SD on his DMS&E contract.

Recent Project Changes

Graduated at End of FY03

- The Science of Localized Corrosion

Started at Beginning of FY04

- Spin-Polarized Transport in Complex Oxides

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Spin-Polarized Transport in Complex Oxides

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Objectives

- *Understand, control and manipulate spin-polarized transport within and between highly spin-polarized oxides in order to create and exploit spintronic functionality.*

Tasks

- Synthesis & Processing: Tailoring Interfacial Chemistry and Structure
- Spin Transport Across and Along Interfaces
- New Theory and Computation Related to Experiments

Participants

- ANL, BNL, LANL, LLNL, ORNL, UI/FS-MRL, Cornell, Univ. of Tennessee

Coordinator

- John Mitchell, ANL, (630) 252-5852, mitchell@anl.gov

Sponsoring/Collaborating Organizations

BES/DMS&E	**DOE/DP**	**Motorola**	**IBM**

Current Center Projects

Start and Graduation Dates

	Start	Graduation
Isolated and Collective Phenomena in Nanocomposite Magnets	FY 00	FY 04
Controlled Defect Structures in Rare-Earth Ba-Cu-O Cuprate Superconductors	FY 00	FY 04
Smart Structures Based on Electroactive Polymers	FY 01	FY 05
Nanoscale Phenomena in Perovskite Thin Films	FY 01	FY 05
Granular Flow and Kinetics	FY 02	FY 06
Synthesis and Processing of Carbon-Based Nanostructured Materials	FY 02	FY 06
Experimental and Computational Lubrication at the Nanoscale	FY 03	FY 07
Spin-Polarized Transport in Complex Oxides	FY 04	FY 08

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Pre-Proposals for New Center Projects

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10 Preproposals were received in response to the call and were reviewed at the 2033 Boston MRS Meeting

- Synthesis and Processing of Novel Reversible Hydrogen Storage Materials
- Atomic-Scale Time-Evolution Phenomena on Corrosion Resistant Alloys
- Defects in Wide Bandgap Semiconductors
- *Functionalization of Nanoporous Materials for Energy and Environmental Applications
- *Structure-Property Relations in Transuranic Compounds
- *High-Field Intermetallic Superconductors
- Hierarchical Self-Assembly
- Processing Science of Nanomaterials
- *Hydrogen Storage in Decorated Doped Carbon Single-Wall Nanotubes
- Relations of Chemical and Mechanical Forces in Dynamic Systems

*** Selected for the final competition**

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CSP's Technology Steering Group (TGS)

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Role of TSG

- Become familiar with the Center's technical activities and comment on their value to DOE Technologies and to industry.
- Provide information from a technology perspective – insight into, and vision of, what is important. Identify technological challenges.
- Influence (steer) the direction of the Center's program. Help develop ideas which can make the Center more effective.
- Take home information and foster closer interactions between the Center, DOE Technologies and industry. Help the Center develop more effective mechanisms for working with DOE Technologies Offices and with industry.
- Become an advocate for, and support the Center's objective to be a model of R and D integration and collaboration within DOE, its Laboratories and with university and industry partners.

2003 TSG Feedback

- The DOE mission connection should be clearly articulated in projects's presentations. But, CSP's emphasis should be on doing good research. Good basic research can be defended on its own.
- CSP should keep an eye on future directions of DOE and OS. It would be interesting to establish links between CSP projects and the Nanoscience Centers.
- The cycle of integration of research results into technology is long (10+ years). Therefore, implementation of research into technology, while good and should remain a long term objective of CSP, should not be a criterion of success for CSP projects.
- Interactions with industry vary from project to project; need to be developed further.
- It is TSG expectations that a project's focus will become sharper in time. We see this, but the project presentations should emphasize the focus and how it has changed in time.

2003 TSG Feedback (Cont.)

- TSG encourages data preservation and documentation from graduated projects. This is an extra added value.
- It is remarkable how effective a “thin layer of glue” has been in bringing people to work together. This is so much more than one would have expected.
- TSG has very positive impressions of CSP and what it is doing. CSP is an excellent model for leverage.
- Spread the story about the success of CSP.

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Research Briefs

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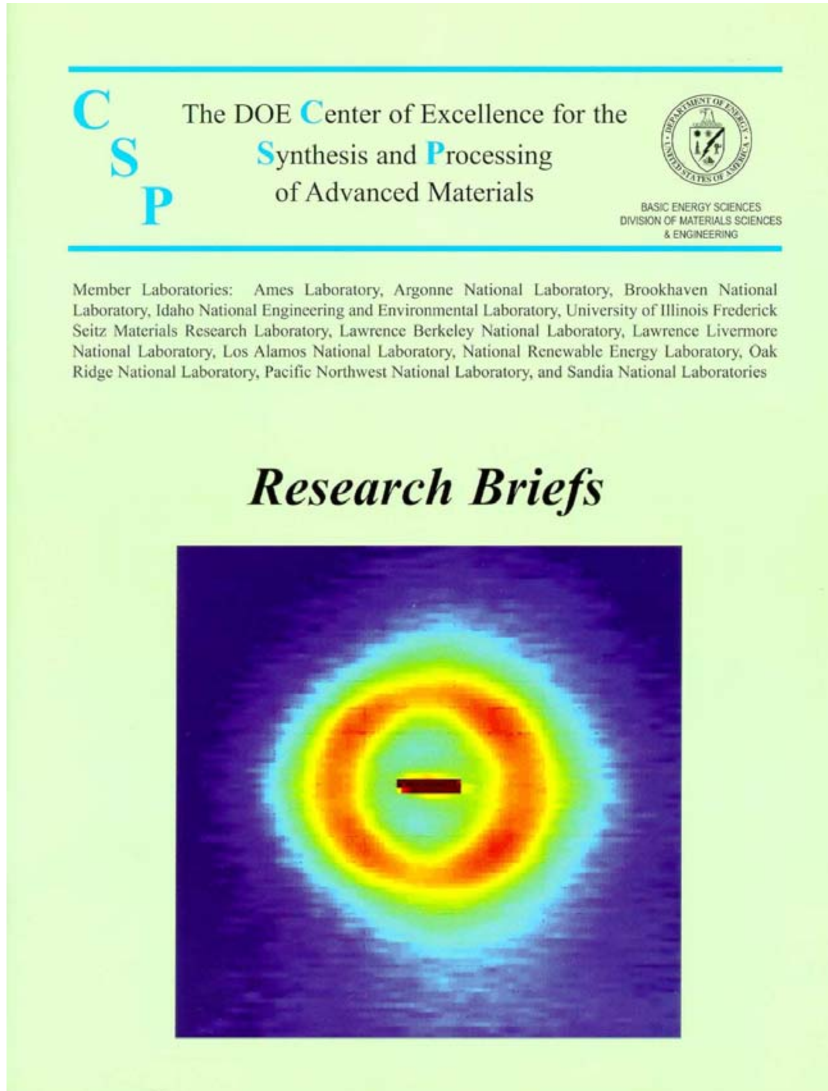
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The DOE Center of Excellence for the Synthesis and Processing of Advanced Materials

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DIVISION OF MATERIALS SCIENCES & ENGINEERING

Member Laboratories: Ames Laboratory, Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Engineering and Environmental Laboratory, University of Illinois Frederick Seitz Materials Research Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories

Research Briefs

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Graduated Project
The Science of Localized Corrosion

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Goal: advance fundamental understanding of localized corrosion of Al to permit accurate life prediction and intelligent design.

Graduated Project

The project addressed three central themes

- *Localized corrosion of aluminum begins with breakdown of the oxide film.*

- *Alloying element segregation and precipitation is known to impact localized corrosion; mechanisms are unknown.*

- *Localized corrosion initiation and propagation are regulated by the interplay between a variety of environmental factors.*

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Graduated Project

Task 1: Structure and Chemistry of the Oxide Film

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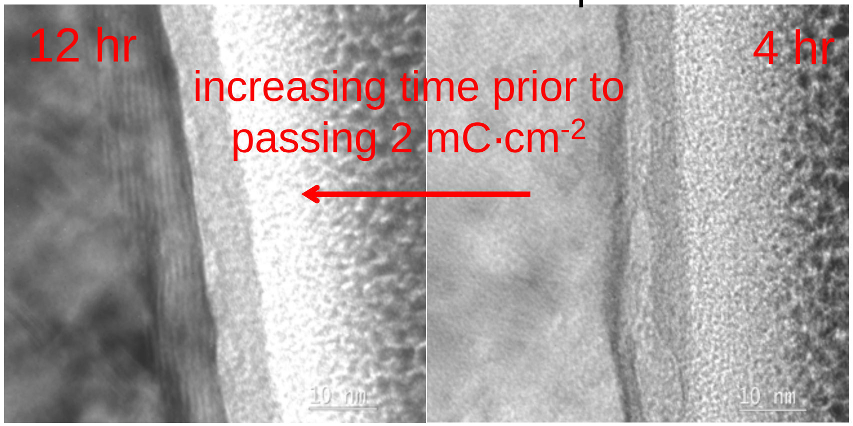
Localized Corrosion of Aluminum begins with Breakdown of the Oxide Film

- Established relationships between the electronic properties, structure, and composition of the oxide film with the mechanism of oxide film breakdown using engineered and native oxides

TEM cross-sections from specific sites



Void nucleation and growth at Al/AlO_x interface

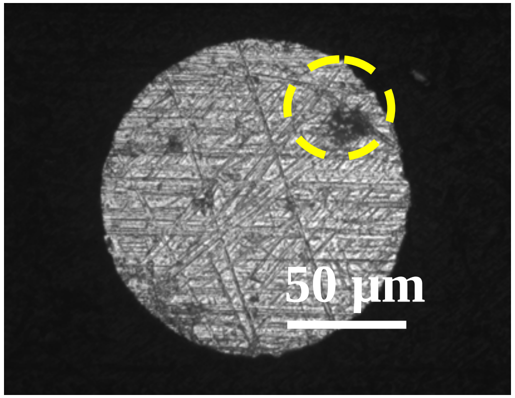
- Unique electrochemical imaging – University of Utah, INEEL
  Micro-electroanalytical and solid state techniques – SNL
  Engineered Oxides and Defect Structures - SNL
  Synthesized Al alloys – Ames Laboratory

Graduated Project
Task 2: Metallurgical Factors

Alloying element segregation and precipitation is known to impact localized corrosion but mechanisms are unknown

- Correlated composition and microstructural heterogeneity with corrosion behavior.
  - Heterogeneity isolation and interrogation
  - Solid solution alloy properties

- Novel micro-electroanalytical techniques – Ohio State University
  Synthesized Al alloys – Ames Laboratory
  Film characterization – PNNL & SNL



Systematic study of Cu, Zn and Mg in Al

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Task 3: Environmental Chemistry and Electrochemistry

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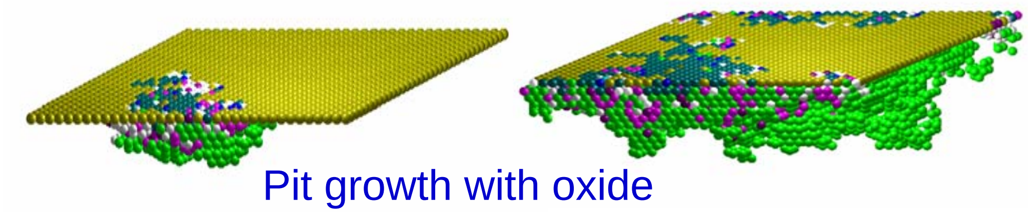
Localized corrosion initiation and propagation are regulated by the interplay between a variety of environmental factors

- Applied modeling (atomistic to continuum level) and experimental (potential, current density, and chemistry mapping) methods to explain how specific corrosion patterns start and evolve.



Pit growth with oxide undercutting

- Modeling at the fundamental level for mesoscale model input – University of Virginia & LLNL
  Mesoscale modeling and system evolution - University of Virginia
  Chemical environment evolution and modeling parameter input –BNL and Ohio State University
  Novel electrochemical experiments simulating localized corrosion – BNL & SNL

Graduated Project

New generation scientists CSP has supported

U. Utah

Irena Serebrennikova, post doc
Chett Boxley
Sungwon Lee

OSU

Ryan Leard, U. Dayton Research Inst.
Jennifer Searles
Yeongsok Kim

UVa

C.D. Taylor

Brookhaven

Hochun Lee, post doc, LG Chemical Ltd.
Kataro Sasaki, post doc, Brookhaven
Vivek Srinivasamurthi – PhD program at Northeastern

Sandia

Kung-Ah Sun – post doc, Jet Propulsion Labs
Craig Johnson – post doc, current

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Graduated Projects - Lessons Learned

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- The most successful projects had sharp focus on one theme with common/similar materials. Fosters cooperation, collaborations, joint publications/presentations.
- Collaborations integrated unique capabilities and expertise.
- Collaborative efforts with universities, industry and others were very relevant and useful.
- Diversity of skills, approaches, and interests among participants present challenges to coordination early on,

  but

  yield opportunities to do/see things differently and add value.
- Face-to-face informal coordination meetings very valuable (~2/yr).
- The "glue" was very valuable in furthering/cementing collaborations.
- Labs' researchers want to be involved in CSP.

After the “Glue” !?!?

A thoughtful input from Laura Lewis (BNL)

- As a veteran of two consecutive (but related) CSP projects, one that has recently graduated, I can say confidently that in our case (“Nanomagnets”) the interactions that formed not only continue on a productive collaborative basis, but also serve as a network in the U.S. magnetic materials community at large. We rely on each other as centers of knowledge for specialized techniques, and to serve on magnetism-related national organizational and programmatic committees. For these reasons, the DOE scientist and their collaborators are considered to exhibit leadership in magnetic materials research.

- I certainly expect that the developed collaborations and interactions will continue for the next few years or so, as long as the individual research objectives remain compatible.

- International meeting program committees (Intermag, MMM) have been filled with DOE scientists who have come to know of each other’s work and expertise as a result of the CSP interaction; staffing of reviewing boards and workshop planning committees have also been filled in this manner. Also, industrial scientist have been directed by one DOE CSP scientist to the relevant work of others by virtue of information exchanged in the course of the CSP interactions.

After the “Glue” !?!?

A thoughtful input from Peggy Hou (LBNL)

- Rowland Cannon (LBNL) worked with Rich Williamson (INEEL) on fracture issues in oxide/alloy systems. One paper is out, and another is in the works.
- I have worked with Jill Wright at INEEL on stress distribution around interfacial pores. Last year, I started working with Boyd Veal at ANL on oxidation stress development and relaxation using in-situ XRD at the APS. This work is on-going and I'm about to deliver a keynote paper on this topic next week.
- My interactions with ORNL, mainly of information and sample exchanges, also benefited from the CSP project. A new collaboration was initiated last month with Kevin McCarty at Sandia, Livermore on surface segregation on some alloys. The purpose is to compare surface segregation to the interface results I've obtained at LBL.
- The CSP project has also brought closer collaborations between Rowland Cannon and myself. We plan to submit a CSP proposal this fall entitled "Relations of Chemical and Mechanical Forces in Dynamic Systems".

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After the “Glue” !?!?

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A thoughtful input from Greg Exharhos (PNNL)

- Eric Peterson (INEEL), Bill Samuels (PNNL), Mira Josowicz (PNNL, now a research professor at Georgia Institute of Technology), ***Phosphazene Membranes for Separation and Speciation***. PI’s were involved with inorganic polymer synthesis by conventional and electropolymerization routes. Collaborative work led to joint laboratory visits, and a follow-on joint proposal to EM regarding sequestration of contaminants from waste streams.
- T.D. Tran and L.R. Hrubesh (LLNL), K. Kinoshita (LBNL), and M.S. Dresselhaus (MIT), ***Processing-Derived Porosity in Carbon Aerogels.*** Dr. Hrubesh moved into a new research area associated with the NIF at LLNL involving Laser interactions with porous solids; he interacts with G.J. Exarhos (PNNL) in this area. GJE chairs a laser damage meeting in which the LLNL researchers are regular participants. The synthesis methods developed in the earlier project are being explored for NIF target development.
- J. McBreen (BNL), E.S. Peterson (INEEL), G.J. Exarhos, W.D. Samuels, J. Liu (now at SNL), ***Engineered Transport Properties in Polymeric Membranes.*** Work led to a joint proposal between BNL and PNNL that was funded through EM and concerned approaches to sequestering ions in polymer membranes.
- Tony Habenschuss (ORNL) and J.G. Curro (SNL), ***Modeling Properties of Polymer Blends.*** PI’s developed PRISM modeling code to understand mixing phenomena in polymer blends. Joint publications resulted. Code used to simulate polymer blend structure in follow-on CSP project (Smart Structures based on Electroactive Polymers). Interactions continue.